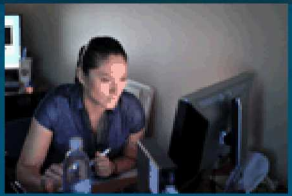
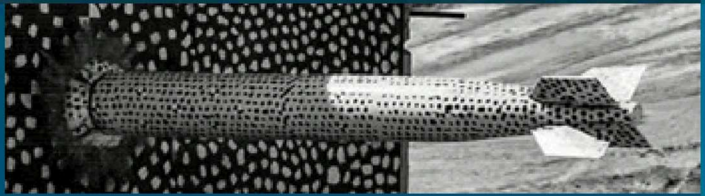
SAND2019-6726C

An Improved Temperature-Dependent Specific Heat Model for Unreacted Explosive Equations of State





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Background

- Accurate temperature computations are critical for simulation hot spot formation and growth to predict sub-detonation response
- Temperature is difficult to calculate in the shock regime
- Temperature is Equation of State (EOS) dependent and a thermodynamically complete EOS provides the most accurate predictions of temperature

Motivation

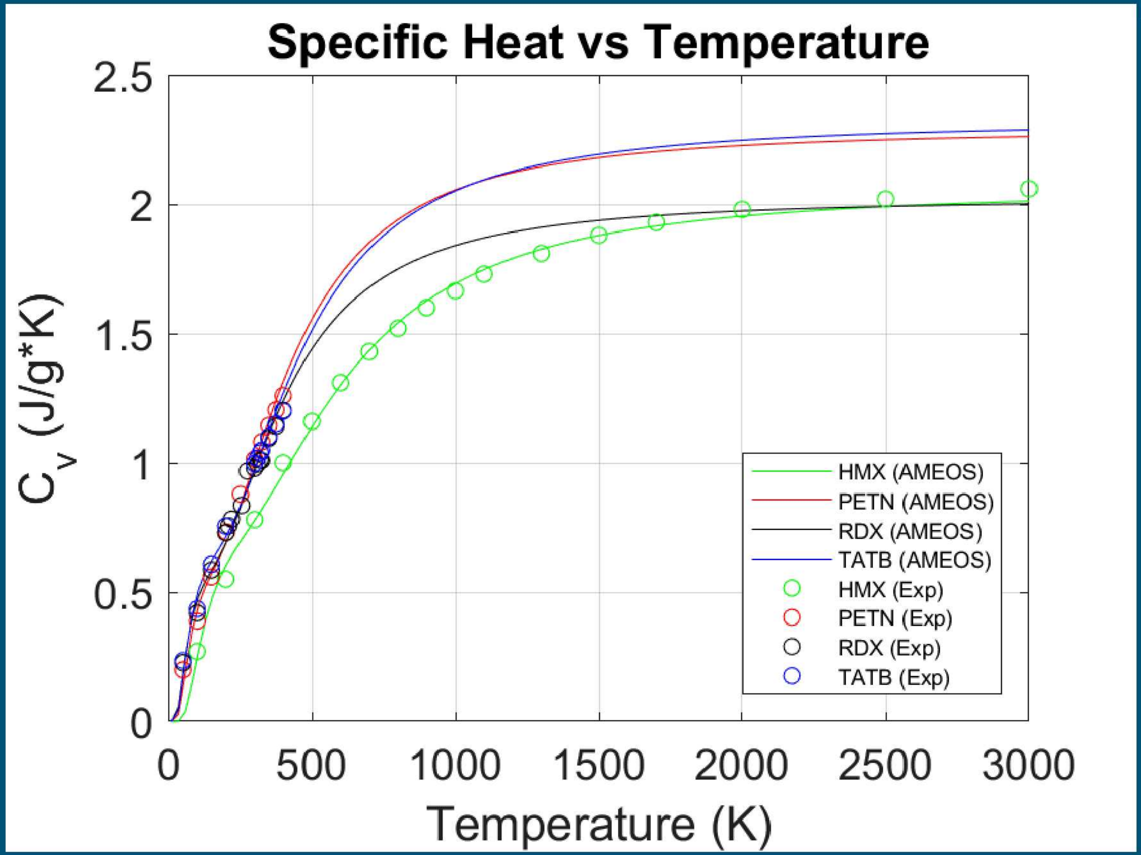
- There is limited thermal EOS data which must be extrapolated to the classic Dulong-Petit limit
- Mesoscale simulation with Arrhenius burn models require thermally physical Equations of State for accurate temperature predictions
- In CTH we desire an improved method to calculate temperature that is physically based as an alternative to the standard Mie-Grüneisen EOS with constant specific heat

Objectives

- Leverage AMEOS model in CTH to incorporate M. R. Baer's Cv(T) data into a more physically based and complete EOS
- Calibrate AMEOS for four unreacted homogeneous explosives (HMX, PETN, RDX, TATB) in temperature-volume space
- Use AMEOS to calculate Hugoniot temperatures for comparison to the temperatures from the standard CTH Mie-Grüneisen EOS

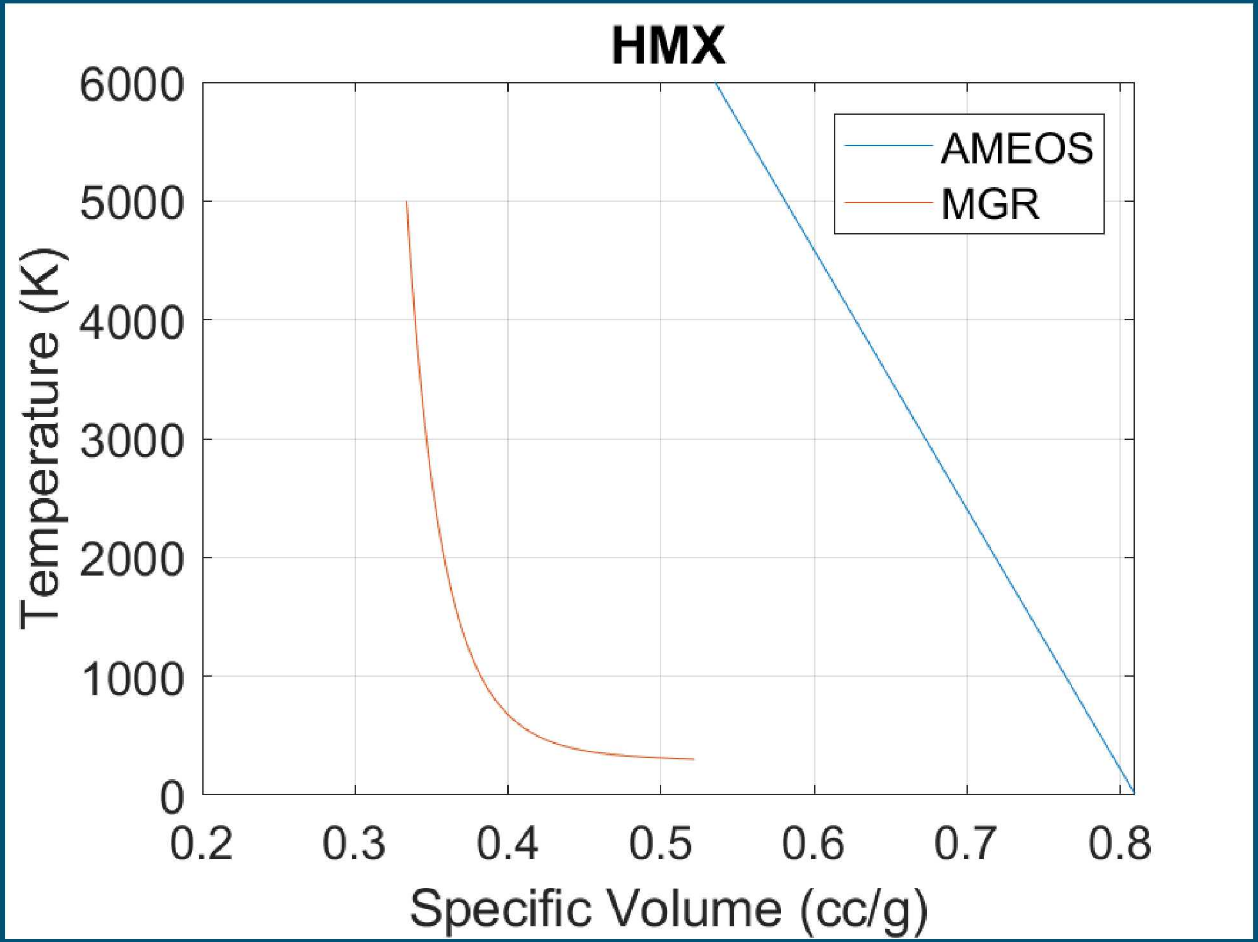
Methods

- Empirical data has been used with the permission of M. R. Baer
- Experiments measured Cp(T), unconfined at 1 atm
- Cv(T) was calculated using the Cp(T) data along with the Grüneisen parameter and coefficient of thermal expansion
- Data is for relatively low temperatures only, due to the reaction in explosive samples
- Low temperature data was curve fit, then extrapolated to an asymptote at the classic limit
- Entire curves were fit using Einstein oscillators
- AMEOS combines Baer's curve fit to experimental data and the hugoniot to give a thermally complete EOS

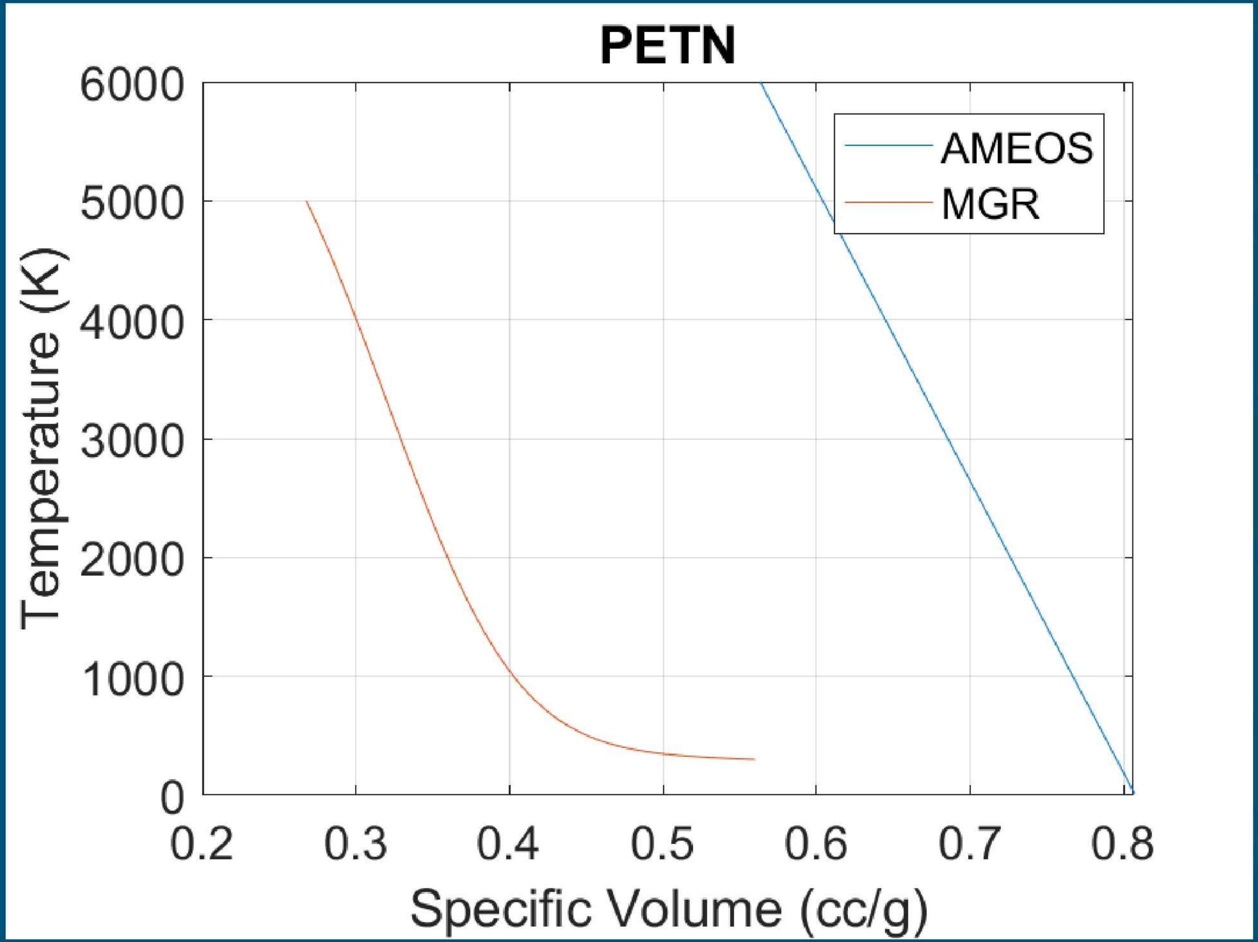


Explosive	Cv1	Th1	Cv2	Th2
HMX	9.64E10	3.49E-2	1.43E11	1.77E-1
PETN	7.99E10	2.09E-2	1.86E11	1.19E-1
RDX	7.7E10	1.79E-2	1.58E11	1.13E-1
TATB	8.53E10	1.93E-2	1.84E11	1.29E-1

Results

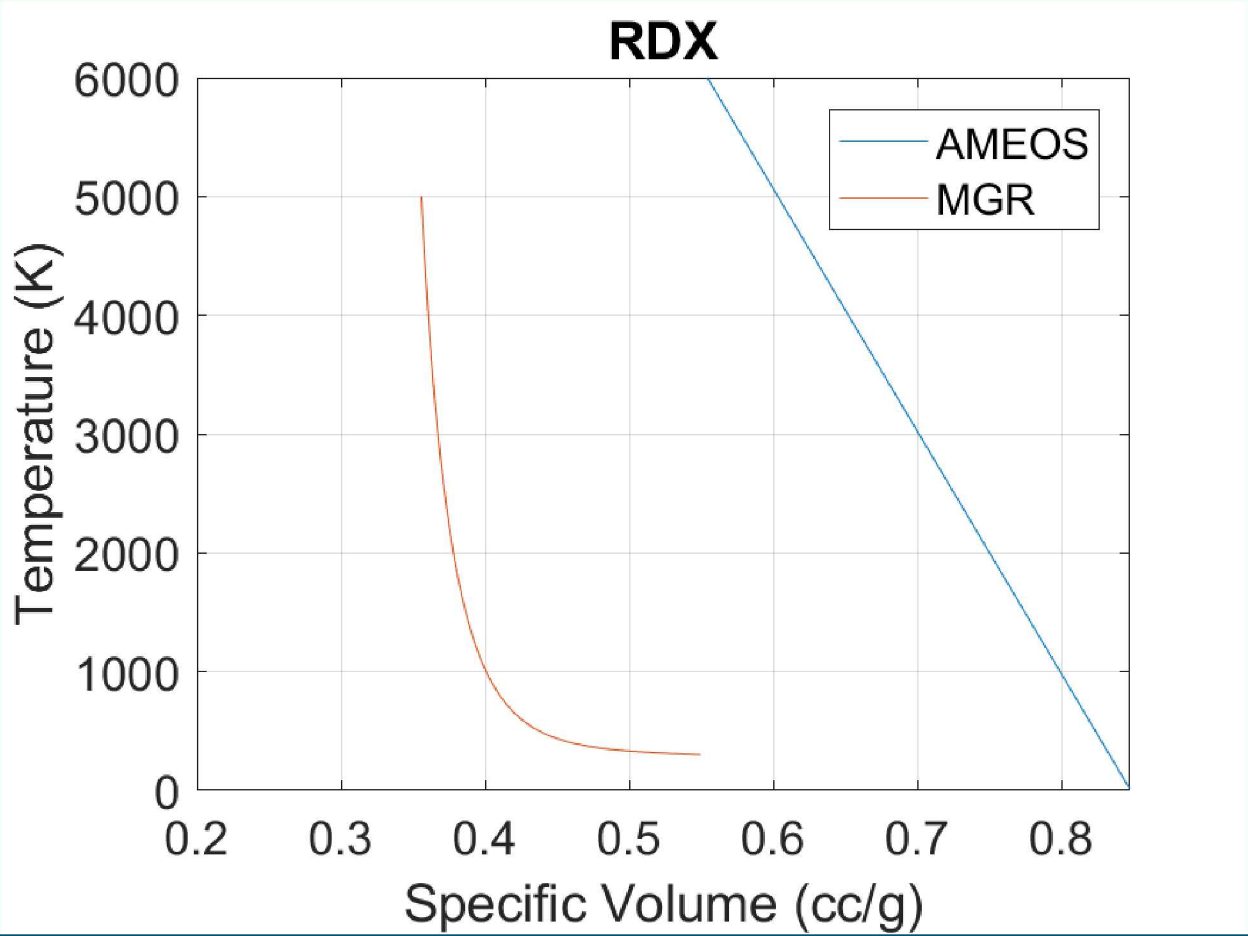


HMX
Temperature (K)
Specific Volume (cc/g)
AMEOS
MGR
0
1000
2000
3000
4000
5000
6000
0.2
0.3
0.4
0.5
0.6
0.7
0.8

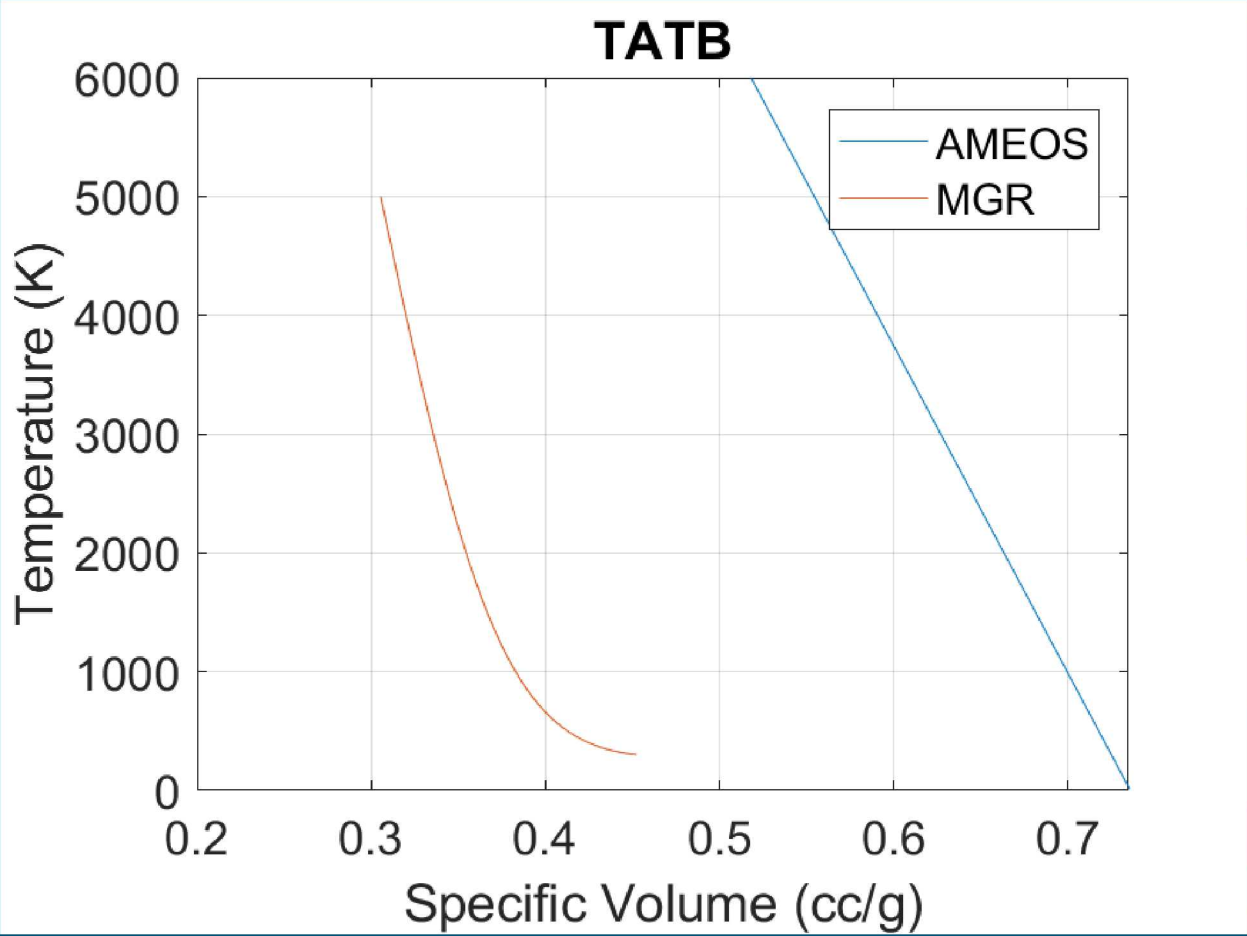


PETN
Temperature (K)
Specific Volume (cc/g)
AMEOS
MGR
0
1000
2000
3000
4000
5000
6000
0.2
0.3
0.4
0.5
0.6
0.7
0.8

Results



RDX
Temperature (K)
Specific Volume (cc/g)
AMEOS
MGR
6000
5000
4000
3000
2000
1000
0
0.2
0.3
0.4
0.5
0.6
0.7
0.8



TATB
Temperature (K)
Specific Volume (cc/g)
AMEOS
MGR
6000
5000
4000
3000
2000
1000
0
0.2
0.3
0.4
0.5
0.6
0.7

Conclusions

- It has been shown that AMEOS can be used to take empirical specific heat data and hugoniots and describe a thermally complete EOS
- AMEOS' complete EOS is more physically based for temperature than the standard Mie-Grüneisen EOS in CTH
- Stretch goal: Talk about T-hug comparison MGR vs AMEOS